wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:00 PM BST

PDB ID	:	4CKH
EMDB ID:	:	EMD-2547
Title	:	Helical reconstruction of ACAP1(BAR-PH domain) decorated membrane tubules by cryo-electron microscopy
Authors	:	Pang, X.Y.; Fan, J.; Zhang, Y.; Zhang, K.; Gao, B.Q.; Ma, J.; Li, J.; Deng, Y.C.; Zhou, Q.J.; Hsu, V.; Sun, F.
Deposited on	:	2014-01-06
Resolution	:	14.00 Å(reported)
Based on PDB ID	:	4NSW

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

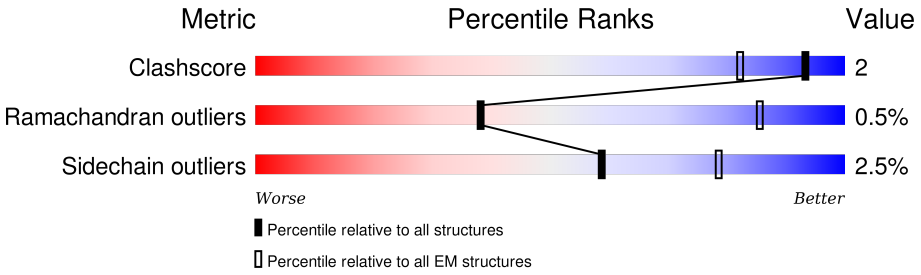
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	382	70% 23% • •
1	B	382	73% 17% 5% 5%
1	C	382	70% 22% • •
1	D	382	73% 17% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11682 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	369	Total	C	N	O	S	0	1
			2941	1841	539	548	13		
1	B	363	Total	C	N	O	S	0	1
			2900	1813	533	541	13		
1	C	369	Total	C	N	O	S	0	1
			2941	1841	539	548	13		
1	D	363	Total	C	N	O	S	0	1
			2900	1813	533	541	13		

There are 20 discrepancies between the modelled and reference sequences:

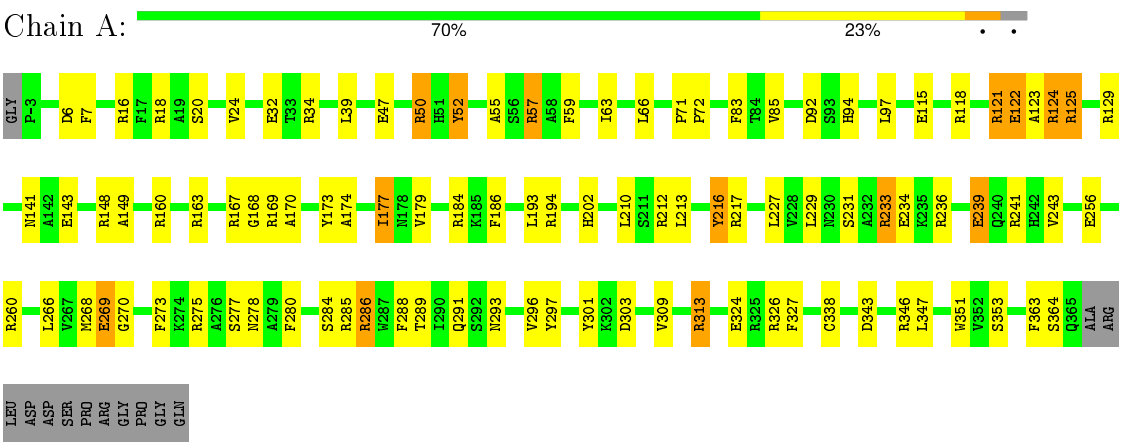
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q15027
A	-3	PRO	-	EXPRESSION TAG	UNP Q15027
A	-2	LEU	-	EXPRESSION TAG	UNP Q15027
A	-1	GLY	-	EXPRESSION TAG	UNP Q15027
A	0	SER	-	EXPRESSION TAG	UNP Q15027
B	-4	GLY	-	EXPRESSION TAG	UNP Q15027
B	-3	PRO	-	EXPRESSION TAG	UNP Q15027
B	-2	LEU	-	EXPRESSION TAG	UNP Q15027
B	-1	GLY	-	EXPRESSION TAG	UNP Q15027
B	0	SER	-	EXPRESSION TAG	UNP Q15027
C	-4	GLY	-	EXPRESSION TAG	UNP Q15027
C	-3	PRO	-	EXPRESSION TAG	UNP Q15027
C	-2	LEU	-	EXPRESSION TAG	UNP Q15027
C	-1	GLY	-	EXPRESSION TAG	UNP Q15027
C	0	SER	-	EXPRESSION TAG	UNP Q15027
D	-4	GLY	-	EXPRESSION TAG	UNP Q15027
D	-3	PRO	-	EXPRESSION TAG	UNP Q15027
D	-2	LEU	-	EXPRESSION TAG	UNP Q15027
D	-1	GLY	-	EXPRESSION TAG	UNP Q15027
D	0	SER	-	EXPRESSION TAG	UNP Q15027

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

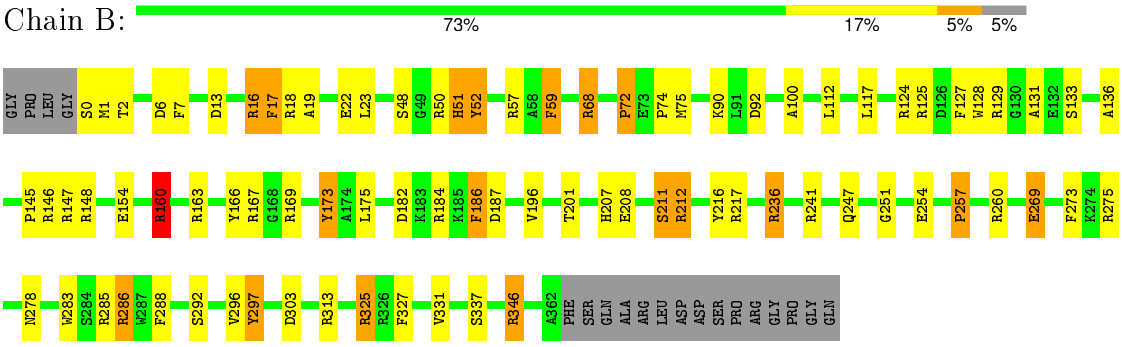
• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain A:



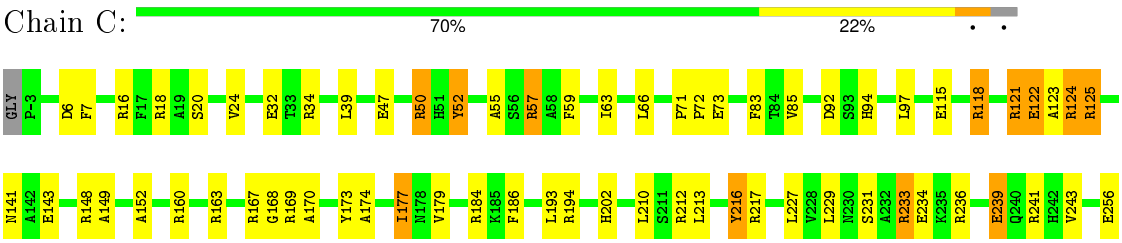
• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

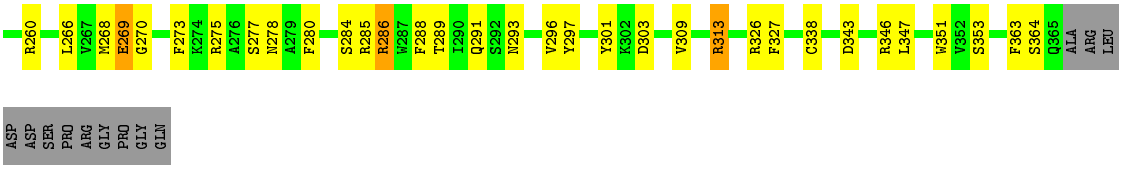
Chain B:



• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

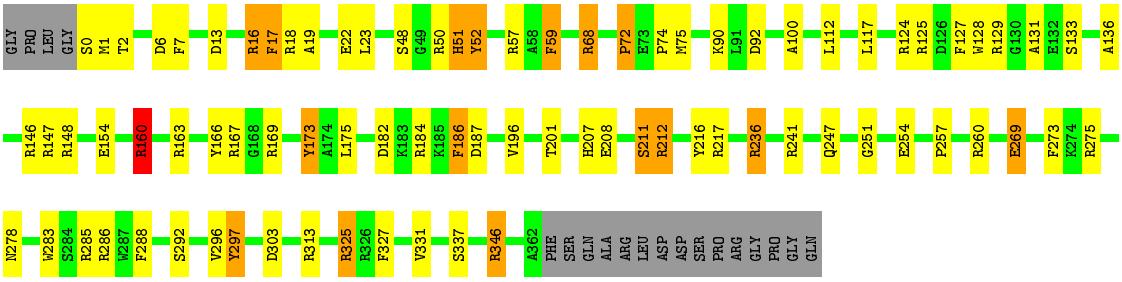
Chain C:





• Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain D:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	GATAN ULTRASCAN4000 CCD CAMERA	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	1.69	26/2990 (0.9%)	2.00	82/4024 (2.0%)
1	B	1.69	19/2947 (0.6%)	2.00	75/3966 (1.9%)
1	C	1.69	27/2990 (0.9%)	2.00	83/4024 (2.1%)
1	D	1.69	20/2947 (0.7%)	2.00	75/3966 (1.9%)
All	All	1.69	92/11874 (0.8%)	2.00	315/15980 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	15
1	C	0	12
1	D	0	15
All	All	0	54

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	SER	CA-CB	8.64	1.66	1.52
1	D	337	SER	CA-CB	8.61	1.65	1.52
1	A	280	PHE	CB-CG	-7.74	1.38	1.51
1	C	280	PHE	CB-CG	-7.69	1.38	1.51
1	A	297	TYR	CG-CD1	7.38	1.48	1.39
1	C	297	TYR	CG-CD1	7.35	1.48	1.39
1	C	239	GLU	CB-CG	7.15	1.65	1.52
1	A	239	GLU	CB-CG	7.09	1.65	1.52
1	B	211	SER	CA-CB	6.93	1.63	1.52
1	D	211	SER	CA-CB	6.88	1.63	1.52
1	C	168	GLY	N-CA	6.77	1.56	1.46
1	A	168	GLY	N-CA	6.73	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CB-CG	6.55	1.64	1.52
1	C	47	GLU	CB-CG	6.54	1.64	1.52
1	A	327	PHE	CG-CD2	6.52	1.48	1.38
1	C	327	PHE	CG-CD2	6.51	1.48	1.38
1	B	146	ARG	CD-NE	6.42	1.57	1.46
1	A	194	ARG	CD-NE	6.42	1.57	1.46
1	D	146	ARG	CD-NE	6.41	1.57	1.46
1	C	194	ARG	CD-NE	6.37	1.57	1.46
1	B	127	PHE	CG-CD1	6.36	1.48	1.38
1	B	48	SER	CA-CB	6.36	1.62	1.52
1	D	127	PHE	CG-CD1	6.35	1.48	1.38
1	D	48	SER	CA-CB	6.33	1.62	1.52
1	C	269	GLU	CG-CD	6.17	1.61	1.51
1	A	269	GLU	CG-CD	6.16	1.61	1.51
1	D	154	GLU	CD-OE1	6.15	1.32	1.25
1	A	285	ARG	CD-NE	6.15	1.56	1.46
1	B	154	GLU	CD-OE1	6.14	1.32	1.25
1	C	285	ARG	CD-NE	6.13	1.56	1.46
1	C	256	GLU	C-N	6.12	1.45	1.34
1	B	22	GLU	CD-OE2	6.08	1.32	1.25
1	A	256	GLU	C-N	6.06	1.45	1.34
1	A	173	TYR	CG-CD1	6.03	1.47	1.39
1	D	254	GLU	CB-CG	5.97	1.63	1.52
1	D	22	GLU	CD-OE2	5.96	1.32	1.25
1	B	254	GLU	CB-CG	5.95	1.63	1.52
1	C	173	TYR	CG-CD1	5.94	1.46	1.39
1	C	301	TYR	CE2-CZ	5.92	1.46	1.38
1	D	288	PHE	CG-CD1	5.89	1.47	1.38
1	B	124	ARG	CD-NE	5.88	1.56	1.46
1	D	124	ARG	CD-NE	5.88	1.56	1.46
1	B	288	PHE	CG-CD1	5.86	1.47	1.38
1	A	301	TYR	CE2-CZ	5.83	1.46	1.38
1	A	270	GLY	CA-C	-5.79	1.42	1.51
1	A	338	CYS	CB-SG	5.77	1.92	1.82
1	C	338	CYS	CB-SG	5.76	1.92	1.82
1	C	270	GLY	CA-C	-5.76	1.42	1.51
1	C	326	ARG	CD-NE	5.75	1.56	1.46
1	A	326	ARG	CD-NE	5.75	1.56	1.46
1	D	133	SER	CA-CB	5.58	1.61	1.52
1	C	286	ARG	CD-NE	5.58	1.55	1.46
1	B	133	SER	CA-CB	5.56	1.61	1.52
1	A	297	TYR	CZ-OH	5.56	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	TYR	CZ-OH	5.55	1.47	1.37
1	B	169	ARG	CD-NE	5.54	1.55	1.46
1	A	286	ARG	CD-NE	5.54	1.55	1.46
1	D	169	ARG	CD-NE	5.49	1.55	1.46
1	A	216	TYR	CE2-CZ	5.46	1.45	1.38
1	C	233	ARG	CD-NE	5.46	1.55	1.46
1	D	74	PRO	CA-CB	5.45	1.64	1.53
1	A	233	ARG	CD-NE	5.43	1.55	1.46
1	C	216	TYR	CE2-CZ	5.42	1.45	1.38
1	B	74	PRO	CA-CB	5.39	1.64	1.53
1	C	123	ALA	CA-CB	5.38	1.63	1.52
1	A	234	GLU	CD-OE1	5.35	1.31	1.25
1	A	123	ALA	CA-CB	5.34	1.63	1.52
1	D	211	SER	CB-OG	5.30	1.49	1.42
1	C	234	GLU	CD-OE1	5.30	1.31	1.25
1	B	211	SER	CB-OG	5.29	1.49	1.42
1	A	72	PRO	N-CA	-5.28	1.38	1.47
1	B	208	GLU	CG-CD	-5.24	1.44	1.51
1	C	72	PRO	N-CA	-5.24	1.38	1.47
1	D	208	GLU	CG-CD	-5.22	1.44	1.51
1	C	167	ARG	CD-NE	5.22	1.55	1.46
1	A	353	SER	CA-CB	5.21	1.60	1.52
1	D	128	TRP	CG-CD1	5.18	1.44	1.36
1	A	167	ARG	CD-NE	5.17	1.55	1.46
1	B	251	GLY	N-CA	-5.17	1.38	1.46
1	C	59	PHE	CG-CD2	5.16	1.46	1.38
1	D	251	GLY	N-CA	-5.15	1.38	1.46
1	C	353	SER	CA-CB	5.15	1.60	1.52
1	A	122	GLU	CG-CD	-5.14	1.44	1.51
1	A	59	PHE	CG-CD2	5.13	1.46	1.38
1	B	128	TRP	CG-CD1	5.13	1.44	1.36
1	B	57	ARG	NE-CZ	5.11	1.39	1.33
1	C	122	GLU	CG-CD	-5.09	1.44	1.51
1	D	236	ARG	CD-NE	5.09	1.55	1.46
1	D	57	ARG	NE-CZ	5.05	1.39	1.33
1	B	236	ARG	CD-NE	5.04	1.55	1.46
1	D	325	ARG	CD-NE	5.03	1.54	1.46
1	C	73	GLU	CD-OE2	5.01	1.31	1.25

All (315) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ARG	NE-CZ-NH1	16.69	128.65	120.30
1	C	163	ARG	NE-CZ-NH1	16.61	128.60	120.30
1	B	50	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	D	50	ARG	NE-CZ-NH2	14.27	127.44	120.30
1	A	18	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	C	18	ARG	NE-CZ-NH2	-14.19	113.21	120.30
1	B	186	PHE	CB-CG-CD2	-13.99	111.01	120.80
1	D	186	PHE	CB-CG-CD2	-13.96	111.03	120.80
1	B	124	ARG	NE-CZ-NH2	-13.41	113.60	120.30
1	D	124	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	C	326	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	A	326	ARG	NE-CZ-NH2	-12.75	113.93	120.30
1	C	217	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	A	217	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	D	288	PHE	CB-CG-CD1	-12.35	112.15	120.80
1	B	288	PHE	CB-CG-CD1	-12.33	112.17	120.80
1	A	57	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	C	57	ARG	NE-CZ-NH2	-12.01	114.29	120.30
1	C	16	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	D	169	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	B	169	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	A	16	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	D	68	ARG	NE-CZ-NH2	11.45	126.03	120.30
1	A	124	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	B	68	ARG	NE-CZ-NH2	11.34	125.97	120.30
1	C	124	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	B	184	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	D	184	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	B	18	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	D	18	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	118	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	D	127	PHE	CB-CG-CD2	-10.69	113.32	120.80
1	B	127	PHE	CB-CG-CD2	-10.67	113.33	120.80
1	D	325	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	D	325	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	B	325	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	C	118	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	B	325	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	184	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	C	184	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	C	217	ARG	NE-CZ-NH2	-10.20	115.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	241	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	C	241	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	B	124	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	D	186	PHE	CB-CG-CD1	9.86	127.70	120.80
1	B	186	PHE	CB-CG-CD1	9.82	127.68	120.80
1	D	124	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	A	18	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	C	18	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	D	212	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	C	326	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	212	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	118	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	D	173	TYR	CB-CG-CD2	-9.14	115.52	121.00
1	A	7	PHE	CB-CG-CD1	-9.10	114.43	120.80
1	C	118	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	326	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	C	7	PHE	CB-CG-CD1	-9.06	114.45	120.80
1	B	173	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	B	297	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	D	297	TYR	CB-CG-CD2	-8.92	115.65	121.00
1	C	148	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	C	169	ARG	NE-CZ-NH1	-8.85	115.87	120.30
1	B	241	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	A	148	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	D	241	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	169	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	A	125	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	313	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	C	313	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	C	125	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	C	301	TYR	CB-CG-CD1	-8.31	116.01	121.00
1	A	163	ARG	NH1-CZ-NH2	-8.30	110.27	119.40
1	A	212	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	301	TYR	CB-CG-CD1	-8.27	116.04	121.00
1	C	163	ARG	NH1-CZ-NH2	-8.21	110.36	119.40
1	B	313	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	D	285	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	6	ASP	CB-CG-OD2	8.06	125.55	118.30
1	B	285	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	212	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	D	313	ARG	NE-CZ-NH2	8.05	124.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	6	ASP	CB-CG-OD2	7.97	125.48	118.30
1	B	7	PHE	CB-CG-CD2	7.87	126.31	120.80
1	D	7	PHE	CB-CG-CD2	7.85	126.30	120.80
1	C	286	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	286	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	127	PHE	CG-CD1-CE1	-7.49	112.56	120.80
1	D	129	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	127	PHE	CG-CD1-CE1	-7.39	112.67	120.80
1	B	129	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	B	288	PHE	CG-CD2-CE2	-7.26	112.81	120.80
1	D	288	PHE	CG-CD2-CE2	-7.19	112.89	120.80
1	B	19	ALA	O-C-N	-7.17	111.22	122.70
1	C	288	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	D	19	ALA	O-C-N	-7.15	111.26	122.70
1	A	288	PHE	CB-CG-CD2	-7.09	115.83	120.80
1	B	346	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	169	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	B	169	ARG	NH1-CZ-NH2	-6.99	111.72	119.40
1	D	346	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	163	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	212	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	182	ASP	CB-CG-OD1	6.93	124.54	118.30
1	B	327	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	B	50	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	B	163	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	68	ARG	NH1-CZ-NH2	-6.90	111.81	119.40
1	A	57	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	D	212	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	D	182	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	288	PHE	CD1-CG-CD2	6.85	127.21	118.30
1	B	160	ARG	N-CA-CB	6.85	122.94	110.60
1	D	327	PHE	CB-CG-CD2	-6.85	116.00	120.80
1	D	50	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	D	160	ARG	N-CA-CB	6.84	122.91	110.60
1	B	187	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	68	ARG	NH1-CZ-NH2	-6.81	111.91	119.40
1	D	288	PHE	CD1-CG-CD2	6.81	127.15	118.30
1	C	275	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	D	187	ASP	CB-CG-OD1	6.76	124.38	118.30
1	C	57	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	234	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	A	275	ARG	NE-CZ-NH2	-6.62	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	100	ALA	O-C-N	-6.60	112.14	122.70
1	A	234	GLU	OE1-CD-OE2	-6.59	115.39	123.30
1	B	100	ALA	O-C-N	-6.58	112.17	122.70
1	B	286	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	286	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	17	PHE	CB-CG-CD2	6.33	125.23	120.80
1	D	17	PHE	CB-CG-CD2	6.32	125.22	120.80
1	A	18	ARG	N-CA-CB	-6.30	99.25	110.60
1	A	212	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	18	ARG	N-CA-CB	-6.29	99.28	110.60
1	C	212	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	52	TYR	CG-CD1-CE1	6.22	126.27	121.30
1	B	52	TYR	CG-CD1-CE1	6.20	126.26	121.30
1	A	266	LEU	CB-CG-CD1	6.20	121.54	111.00
1	C	149	ALA	CB-CA-C	-6.19	100.82	110.10
1	A	83	PHE	CB-CG-CD1	6.18	125.12	120.80
1	A	149	ALA	CB-CA-C	-6.18	100.84	110.10
1	B	269	GLU	N-CA-CB	6.17	121.71	110.60
1	D	269	GLU	N-CA-CB	6.17	121.70	110.60
1	A	16	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	266	LEU	CB-CG-CD1	6.15	121.46	111.00
1	A	273	PHE	CB-CG-CD2	-6.15	116.50	120.80
1	A	39	LEU	CB-CA-C	-6.14	98.53	110.20
1	C	83	PHE	CB-CG-CD1	6.14	125.10	120.80
1	C	141	ASN	O-C-N	-6.14	112.88	122.70
1	A	167	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	285	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	275	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	39	LEU	CB-CA-C	-6.12	98.58	110.20
1	A	141	ASN	O-C-N	-6.11	112.92	122.70
1	C	167	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	201	THR	CA-CB-CG2	-6.11	103.85	112.40
1	D	201	THR	CA-CB-CG2	-6.10	103.86	112.40
1	A	167	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	A	268	MET	CG-SD-CE	-6.10	90.45	100.20
1	B	303	ASP	N-CA-CB	-6.08	99.65	110.60
1	C	268	MET	CG-SD-CE	-6.07	90.48	100.20
1	C	273	PHE	CB-CG-CD2	-6.07	116.55	120.80
1	D	303	ASP	N-CA-CB	-6.07	99.67	110.60
1	C	16	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	13	ASP	CB-CA-C	6.00	122.41	110.40
1	C	72	PRO	CA-N-CD	6.00	120.09	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	13	ASP	CB-CA-C	5.99	122.39	110.40
1	A	72	PRO	CA-N-CD	5.98	120.07	111.70
1	D	275	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	285	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	117	LEU	CB-CG-CD2	5.93	121.08	111.00
1	C	63	ILE	N-CA-CB	5.92	124.42	110.80
1	B	117	LEU	CB-CG-CD2	5.89	121.02	111.00
1	A	63	ILE	N-CA-CB	5.89	124.34	110.80
1	B	182	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	D	72	PRO	N-CA-CB	-5.88	96.13	102.60
1	C	167	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	B	72	PRO	N-CA-CB	-5.87	96.14	102.60
1	B	216	TYR	CD1-CE1-CZ	-5.87	114.52	119.80
1	C	297	TYR	CZ-CE2-CD2	5.86	125.08	119.80
1	C	184	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	216	TYR	CD1-CE1-CZ	-5.85	114.53	119.80
1	C	347	LEU	CB-CG-CD1	5.83	120.91	111.00
1	A	297	TYR	CZ-CE2-CD2	5.79	125.01	119.80
1	D	182	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	347	LEU	CB-CG-CD1	5.79	120.84	111.00
1	A	184	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	59	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	B	131	ALA	N-CA-CB	-5.74	102.06	110.10
1	D	52	TYR	CD1-CE1-CZ	-5.73	114.65	119.80
1	D	59	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	D	131	ALA	N-CA-CB	-5.68	102.14	110.10
1	A	186	PHE	CB-CG-CD1	5.68	124.78	120.80
1	C	186	PHE	CB-CG-CD1	5.65	124.75	120.80
1	C	52	TYR	CB-CG-CD1	5.65	124.39	121.00
1	A	52	TYR	CB-CG-CD1	5.62	124.37	121.00
1	B	52	TYR	CD1-CE1-CZ	-5.62	114.74	119.80
1	A	256	GLU	N-CA-CB	-5.59	100.53	110.60
1	D	296	VAL	CA-CB-CG2	5.59	119.29	110.90
1	B	147	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	124	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	296	VAL	CA-CB-CG2	5.57	119.25	110.90
1	C	256	GLU	N-CA-CB	-5.54	100.62	110.60
1	C	278	ASN	O-C-N	-5.53	113.85	122.70
1	B	2	THR	CA-CB-CG2	-5.53	104.66	112.40
1	A	278	ASN	O-C-N	-5.52	113.87	122.70
1	A	293	ASN	CB-CA-C	5.52	121.44	110.40
1	A	273	PHE	CB-CG-CD1	5.51	124.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	293	ASN	CB-CA-C	5.51	121.43	110.40
1	D	147	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	20	SER	N-CA-CB	5.50	118.75	110.50
1	B	175	LEU	CB-CG-CD1	5.50	120.34	111.00
1	D	273	PHE	CB-CG-CD2	5.49	124.65	120.80
1	B	166	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	C	20	SER	N-CA-CB	5.49	118.73	110.50
1	D	166	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	D	2	THR	CA-CB-CG2	-5.48	104.72	112.40
1	B	297	TYR	CB-CG-CD1	5.47	124.28	121.00
1	D	175	LEU	CB-CG-CD1	5.46	120.29	111.00
1	C	173	TYR	CB-CG-CD1	5.46	124.28	121.00
1	C	297	TYR	CD1-CE1-CZ	5.46	124.71	119.80
1	C	273	PHE	CB-CG-CD1	5.45	124.62	120.80
1	A	297	TYR	CD1-CE1-CZ	5.44	124.70	119.80
1	B	273	PHE	CB-CG-CD2	5.43	124.60	120.80
1	C	124	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	297	TYR	CB-CG-CD1	5.42	124.25	121.00
1	D	16	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	343	ASP	O-C-N	-5.42	114.03	122.70
1	A	343	ASP	O-C-N	-5.41	114.04	122.70
1	B	16	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	C	50	ARG	CG-CD-NE	-5.40	100.45	111.80
1	A	50	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	92	ASP	CB-CG-OD1	5.39	123.15	118.30
1	D	136	ALA	O-C-N	-5.39	114.08	122.70
1	D	51	HIS	N-CA-CB	5.38	120.28	110.60
1	C	92	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	136	ALA	O-C-N	-5.34	114.15	122.70
1	A	167	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	B	51	HIS	N-CA-CB	5.34	120.22	110.60
1	A	303	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	313	ARG	N-CA-CB	-5.33	101.00	110.60
1	D	75	MET	O-C-N	-5.33	114.17	122.70
1	C	291	GLN	N-CA-CB	5.31	120.16	110.60
1	D	313	ARG	N-CA-CB	-5.31	101.04	110.60
1	C	174	ALA	N-CA-CB	-5.30	102.68	110.10
1	B	57	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	346	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	174	ALA	N-CA-CB	-5.29	102.69	110.10
1	B	75	MET	O-C-N	-5.29	114.23	122.70
1	C	303	ASP	CB-CG-OD2	-5.29	113.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	297	TYR	CG-CD1-CE1	-5.29	117.07	121.30
1	A	291	GLN	N-CA-CB	5.29	120.11	110.60
1	A	363	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	D	92	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	92	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	346	ARG	CD-NE-CZ	5.26	130.96	123.60
1	D	57	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	170	ALA	N-CA-CB	5.25	117.45	110.10
1	A	173	TYR	CB-CG-CD1	5.25	124.15	121.00
1	C	363	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	B	297	TYR	CG-CD1-CE1	-5.23	117.12	121.30
1	D	6	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	52	TYR	CZ-CE2-CD2	5.22	124.50	119.80
1	C	167	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	C	170	ALA	N-CA-CB	5.21	117.39	110.10
1	C	227	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	52	TYR	CZ-CE2-CD2	5.20	124.48	119.80
1	C	284	SER	N-CA-CB	5.20	118.29	110.50
1	A	227	LEU	CB-CG-CD2	5.19	119.82	111.00
1	C	179	VAL	O-C-N	-5.19	114.40	122.70
1	D	50	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	284	SER	N-CA-CB	5.18	118.27	110.50
1	C	85	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	C	210	LEU	CB-CA-C	5.17	120.03	110.20
1	A	85	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	C	231	SER	N-CA-CB	-5.17	102.74	110.50
1	B	50	ARG	CG-CD-NE	-5.17	100.94	111.80
1	C	177	ILE	O-C-N	-5.17	114.43	122.70
1	A	177	ILE	O-C-N	-5.17	114.43	122.70
1	C	160	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	55	ALA	C-N-CA	5.16	134.59	121.70
1	B	292	SER	N-CA-CB	5.16	118.23	110.50
1	C	55	ALA	C-N-CA	5.14	134.56	121.70
1	B	6	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	210	LEU	CB-CA-C	5.13	119.96	110.20
1	A	179	VAL	O-C-N	-5.13	114.49	122.70
1	A	231	SER	N-CA-CB	-5.13	102.81	110.50
1	D	283	TRP	CG-CD2-CE3	-5.10	129.31	133.90
1	C	278	ASN	CA-CB-CG	-5.10	102.17	113.40
1	D	173	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	B	173	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	D	292	SER	N-CA-CB	5.09	118.14	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	90	LYS	CB-CA-C	5.09	120.58	110.40
1	A	278	ASN	CA-CB-CG	-5.07	102.24	113.40
1	B	90	LYS	CB-CA-C	5.07	120.54	110.40
1	A	256	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	D	52	TYR	CB-CA-C	5.06	120.52	110.40
1	A	351	TRP	CG-CD2-CE3	-5.06	129.35	133.90
1	B	52	TYR	CB-CA-C	5.06	120.51	110.40
1	A	160	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	193	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	C	121	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	C	351	TRP	CG-CD2-CE3	-5.05	129.36	133.90
1	C	193	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	C	152	ALA	N-CA-CB	-5.04	103.05	110.10
1	D	23	LEU	N-CA-CB	-5.04	100.33	110.40
1	C	256	GLU	OE1-CD-OE2	-5.03	117.27	123.30
1	A	121	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	B	283	TRP	CG-CD2-CE3	-5.02	129.38	133.90
1	D	173	TYR	CG-CD1-CE1	-5.02	117.28	121.30
1	B	23	LEU	N-CA-CB	-5.02	100.36	110.40
1	B	128	TRP	CH2-CZ2-CE2	5.02	122.42	117.40
1	C	7	PHE	CB-CG-CD2	5.00	124.30	120.80
1	A	141	ASN	CA-C-O	5.00	130.60	120.10

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLU	Peptide
1	A	124	ARG	Sidechain
1	A	202	HIS	Sidechain
1	A	216	TYR	Sidechain
1	A	236	ARG	Sidechain
1	A	286	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	50	ARG	Sidechain
1	A	52	TYR	Sidechain
1	A	57	ARG	Sidechain
1	A	71	PRO	Peptide
1	B	125	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	16	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	160	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	17	PHE	Sidechain
1	B	173	TYR	Sidechain
1	B	186	PHE	Sidechain
1	B	212	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	346	ARG	Sidechain
1	B	51	HIS	Sidechain
1	B	52	TYR	Sidechain
1	B	59	PHE	Sidechain
1	B	68	ARG	Sidechain
1	C	115	GLU	Peptide
1	C	124	ARG	Sidechain
1	C	202	HIS	Sidechain
1	C	216	TYR	Sidechain
1	C	236	ARG	Sidechain
1	C	286	ARG	Sidechain
1	C	313	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	50	ARG	Sidechain
1	C	52	TYR	Sidechain
1	C	57	ARG	Sidechain
1	C	71	PRO	Peptide
1	D	125	ARG	Sidechain
1	D	148	ARG	Sidechain
1	D	16	ARG	Sidechain
1	D	160	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	17	PHE	Sidechain
1	D	173	TYR	Sidechain
1	D	186	PHE	Sidechain
1	D	212	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	346	ARG	Sidechain
1	D	51	HIS	Sidechain
1	D	52	TYR	Sidechain
1	D	59	PHE	Sidechain
1	D	68	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2941	0	2956	12	0
1	B	2900	0	2921	23	0
1	C	2941	0	2957	11	0
1	D	2900	0	2921	21	0
All	All	11682	0	11755	40	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:NH2	1:D:247:GLN:HB2	1.33	1.39
1:B:236:ARG:NH2	1:D:247:GLN:CB	1.92	1.30
1:B:236:ARG:HH21	1:D:247:GLN:CA	1.48	1.27
1:B:247:GLN:HB2	1:D:236:ARG:NH2	1.49	1.27
1:B:247:GLN:CA	1:D:236:ARG:HH21	1.57	1.17
1:B:236:ARG:HH21	1:D:247:GLN:HA	1.02	1.15
1:B:247:GLN:CB	1:D:236:ARG:NH2	2.09	1.15
1:B:247:GLN:HA	1:D:236:ARG:HH21	1.06	1.10
1:B:247:GLN:CA	1:D:236:ARG:NH2	2.25	0.98
1:B:236:ARG:NH2	1:D:247:GLN:CA	2.18	0.96
1:B:247:GLN:HB2	1:D:236:ARG:HH22	1.28	0.87
1:B:236:ARG:HH22	1:D:247:GLN:HB2	1.09	0.86
1:B:247:GLN:HA	1:D:236:ARG:NH2	1.91	0.83
1:B:236:ARG:NH2	1:D:247:GLN:HA	1.88	0.83
1:A:122:GLU:OE1	1:C:122:GLU:OE1	2.16	0.64
1:B:236:ARG:NH2	1:D:247:GLN:CG	2.67	0.54
1:A:125:ARG:NH2	1:C:125:ARG:NH2	2.57	0.52
1:A:129:ARG:CD	1:C:118:ARG:NE	2.72	0.51
1:A:239:GLU:O	1:A:243:VAL:HG23	2.12	0.49
1:C:229:LEU:HD21	1:C:233:ARG:NH2	2.27	0.49
1:C:239:GLU:O	1:C:243:VAL:HG23	2.12	0.49
1:A:229:LEU:HD21	1:A:233:ARG:NH2	2.28	0.48
1:B:236:ARG:HH21	1:D:247:GLN:CB	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HD2	1:C:118:ARG:HE	1.82	0.45
1:B:247:GLN:N	1:D:236:ARG:NH2	2.64	0.45
1:A:213:LEU:HD21	1:B:196:VAL:HG13	2.00	0.44
1:C:213:LEU:HD21	1:D:196:VAL:HG13	1.99	0.43
1:B:207:HIS:CE1	1:B:211:SER:HB2	2.54	0.43
1:D:207:HIS:CE1	1:D:211:SER:HB2	2.54	0.42
1:B:236:ARG:CZ	1:D:247:GLN:HG3	2.50	0.42
1:A:289:THR:O	1:A:296:VAL:HG22	2.20	0.42
1:C:32:GLU:CD	1:C:121:ARG:HH12	2.23	0.42
1:A:94:HIS:O	1:A:97:LEU:HB3	2.20	0.42
1:C:289:THR:O	1:C:296:VAL:HG22	2.20	0.41
1:A:32:GLU:CD	1:A:121:ARG:HH12	2.23	0.41
1:B:286:ARG:HA	1:B:286:ARG:HD3	1.96	0.41
1:C:143:GLU:CD	1:D:325:ARG:HH12	2.24	0.41
1:A:143:GLU:CD	1:B:325:ARG:HH12	2.24	0.41
1:A:324:GLU:O	1:B:145:PRO:HA	2.22	0.40
1:C:94:HIS:O	1:C:97:LEU:HB3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	46	83
1	B	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	24	69
1	C	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	46	83
1	D	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	24	69
All	All	1456/1528 (95%)	1402 (96%)	46 (3%)	8 (0%)	38	77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	SER
1	C	364	SER
1	B	278	ASN
1	D	278	ASN
1	B	257	PRO
1	D	257	PRO
1	B	72	PRO
1	D	72	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/325 (97%)	308 (98%)	7 (2%)	60	83
1	B	311/325 (96%)	302 (97%)	9 (3%)	50	78
1	C	315/325 (97%)	308 (98%)	7 (2%)	60	83
1	D	311/325 (96%)	303 (97%)	8 (3%)	54	80
All	All	1252/1300 (96%)	1221 (98%)	31 (2%)	59	81

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	66	LEU
1	A	177	ILE
1	A	260	ARG
1	A	269	GLU
1	A	277	SER
1	A	309	VAL
1	B	0	SER
1	B	1	MET
1	B	112	LEU
1	B	160	ARG
1	B	257	PRO
1	B	260	ARG
1	B	269	GLU

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Mol	Chain	Res	Type
1	B	297	TYR
1	B	331	VAL
1	C	24	VAL
1	C	66	LEU
1	C	177	ILE
1	C	260	ARG
1	C	269	GLU
1	C	277	SER
1	C	309	VAL
1	D	0	SER
1	D	1	MET
1	D	112	LEU
1	D	160	ARG
1	D	260	ARG
1	D	269	GLU
1	D	297	TYR
1	D	331	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	HIS
1	D	207	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.